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Magnetic polarons in materials with colossal magnetoresistance

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Abstract

We construct a phase diagram for the materials with colossal magnetoresistance. The basic model which describes these materials is a double-exchange model. We rigorously prove that a ground state of this model corresponds to a phase-separated state with small ferromagnetic polarons inside an antiferromagnetic matrix. The general picture of a percolative state, which emerges from our calculations, is in good agreement with recent experiments on doped manganites.

Keywords: Colossal magnetoresistance; Double exchange; Strongly correlated electrons

Recent beautiful experiments on electron transport [1], NMR [2] and neutron scattering [3] strongly support a picture of phase-separated ground state in doped manganites. This state was also advocated in recent numerical investigations [4]. In the present paper we provide a coherent theoretical confirmation of this picture, proving that a polaronic phase-separated ground state corresponds to a global minimum of the energy in our system.

We consider the double-exchange model [5] with the Hamiltonian

$$H = -t\sum_{\langle i,j\rangle}(c^\dagger_{i,\sigma}c_{i,\sigma} + \text{h.c.}) - J_\mathrm{H}\sum_i \boldsymbol{S}_i\sigma_i + J_\mathrm{ff}\sum_{\langle i,j\rangle}\boldsymbol{S}_i\boldsymbol{S}_j, \tag{1}$$

where J_H is the on-site FM exchange and J_ff is the AFM Heisenberg exchange. We work in the limit of large Hund's coupling: $J_\mathrm{H}S \gg zt \gg J_\mathrm{ff}S^2$.

We calculate at first an energy of homogeneous state as a function of the carrier's concentration x. We obtain that for $x < x_{\mathrm{C}1} = (8\pi^4/3)(J_\mathrm{ff}(2S+1)^{3/2}/zt)^3$ a collinear AFM-state is realized [6,7].

For $x_{\mathrm{C}1} < x < x_{\mathrm{C}2} \approx 13.5x_{\mathrm{C}1}$ a quantum two-band canted state arises in the system [8], while for $x_{\mathrm{C}2} < x < x_{\mathrm{C}3} = (8J_\mathrm{ff}S\sqrt{2S+1})/t$ a quantum one-band canted state takes place [8]. For $x > x_{\mathrm{C}3}$ a quantum one-band canting transforms to a classical canting of De-Gennes type with an energy [5]:

$$E_\mathrm{clas.cant} = -J_\mathrm{H}\frac{S}{2}x - \frac{zt^2x^2}{2J_\mathrm{ff}} - \frac{z}{2}J_\mathrm{ff}S^2. \tag{2}$$

Finally for $x > x_{\mathrm{C}4} = 2J_\mathrm{ff}S^2/t$ a collinear FM state is realized in the system [5].

Let us now verify a homogeneous state on the instability towards phase separation. For $x < x_{\mathrm{C}1}$ the compressibility of the system $\kappa^2 = \mathrm{d}^2E/\mathrm{d}x^2$ is positive. However for $x_{\mathrm{C}1} < x < x_{\mathrm{C}4}$ the compressibility changes its sign and becomes negative. Especially simple is the expression for the compresibility for $x_{\mathrm{C}3} < x < x_{\mathrm{C}4}$, where a canted state becomes classical:

$$\kappa^2 = -\frac{zt^2}{J_\mathrm{ff}S^2} < 0. \tag{3}$$

So, while collinear AFM and FM states at least correspond to a local minimum of an energy, a canted state is absolutely unstable. This fact reflects a tendency towards phase separation in the system. We can show that the most energetically benefitial phase-separated state corresponds to FM-polarons embedded into an

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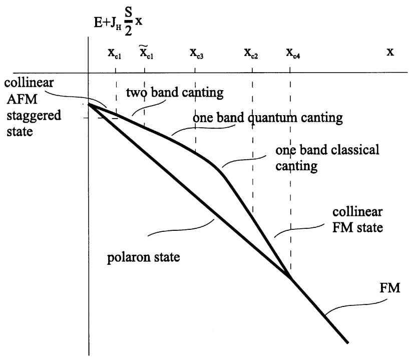

Fig. 1. Phase diagram of the double-exchange model.

AFM-matrix. To show this let us calculate an energy of a polaron state, assuming that each polaron is formed by one conduction electron localized inside a FM-bubble. A polaron energy for a spherical shape of a bubble reads [7–9]:

$$E_{\mathrm{pol}} = -J_{\mathrm{H}}\frac{S}{2}x - ztx + \frac{5\pi}{3}x(\pi t)^{3/5}(2zJ_{\mathrm{ff}}S^2)^{2/5} - J_{\mathrm{ff}}\frac{zS^2}{2}. \quad (4)$$

Note that in a layered situation FM-polarons have an ellipsoidal shape [10].

A direct comparison of the energies of a homogeneous state and a polaron state shows, that an energy of a polaron state corresponds to a global minimum of energy for all concentrations $0 < x < x_{C5}$. Note that at $x = x_{C5} = 3/4\pi(a/R_{\mathrm{pol}})^3 = 3/4\pi(2zJ_{\mathrm{ff}}S^2/\pi t)^{3/5}$ the polarons start to overlap and all the sample becomes ferromagnetic. The resulting phase diagram of the double-exchange model is presented in Fig. 1.

In conclusion we have shown that the tendency towards a phase separation and a formation of a spatially inhomogeneous percolative state [11] is an inherent property of the double-exchange model.

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